Quantitative Photoacoustic Imaging of Chlorophyll Using a GPU-Accelerated Finite Element Method

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Abstract. Chlorophyll in leaves is tightly associated with physiological status of plants. Chemical extraction or hyperspectral estimation is the conventional method to estimate the concentration of Chlorophyll in leaves. However, chemical extraction is invasive and time consuming, and hyperspectral method is extremely sensitive to background light. In this paper, we develop a quantitative photoacoustic imaging technique based on a finite-element-based reconstruction algorithm accelerated by a multicore GPU card to image morphological features and derive distribution of Chlorophyll A in rice leaves. The results suggest that this new method holds great potential in various studies of plant physiology.

AMS subject classifications: 65N30, 65Y05

Key words: Photoacoustic tomography, finite element method, GPU-acceleration, chlorophyll.

1 Introduction

There are three major types of pigments in most plants: chlorophyll, carotenoid and anthocyanin. The primary function of these pigments is photosynthesis, which is largely

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responsible for oxygen supply for life on the earth [1,2]. Photosynthesis converts solar energy into chemical energy which supports the activities of organisms. Chlorophyll plays a key role in photosynthesis due to its strong light absorbing capability [3–5]. Several methods have already been used to estimate the content of chlorophyll in leaves including chemical extraction, spectrophotometric measurement, and high performance liquid chromatography [6–8]. However, all of these procedures are time-consuming and invasive, making it impossible to monitor the longitudinal variations of the chlorophyll [9].

As a non-invasive method, hyperspectral measurement is capable of deriving accurate chlorophyll content in a leaf by analyzing its reflectance spectra [10]. Unfortunately, it is extremely sensitive to background light, and thus requires a dark room to avoid noise from outer light sources, which makes it challenging for outdoor use [11]. Photoacoustic imaging (PAI) is an emerging noninvasive imaging technique that combines the merits of rich optical contrast and high acoustic resolution in a single modality [12]. Comparing to hyperspectral measurement, PAI is not sensitive to background light and holds the potential for outdoor use. In PAI, photon absorption of nanosecond laser pulses by the target leads to rapid thermal expansion and generates wideband photoacoustic waves, which are detected to produce images. PAI has been extensively applied in the fields of biology and medicine [13–16]. Photoacoustic computed tomography (PACT), a reconstruction-based modality, utilizes an area illumination and scans flat acoustic transducers to obtain multiple detections for image reconstruction [17]. Although the spatial resolution is lower than photoacoustic microscopy, it has a large field of view (FOV), a deep penetration depth and a high imaging speed. In addition, apart from photoacoustic microscopy which is reconstructed by directly back-projecting the depth-resolved photoacoustic signals, PACT is able to derive absolute absorption coefficients of targets using model-based quantitative reconstruction methods [18–20]. Commonly, in quantitative PACT reconstruction, the generation and propagation of photoacoustic waves in targets is described using Helmholtz-like photoacoustic wave equation, and the photon diffusion equation which is the first-order approximation to the rigorous radiative transfer equation is used to depict the light distribution. By using finite element method (FEM), the quantitative reconstruction algorithms have been developed and extensively applied in breast cancer detection, arthritis diagnosis, and brain investigation [21]. Previously, we proposed a time domain based FEM method to solve the partial differential equations, which provides better image quality with much more accurately recovered value and less artifacts compared to its frequency domain counterpart [22]. However, the time domain approach is extremely time consuming, which usually requires dozens of hours reconstruct a two-dimensional PACT image with a typical mesh size. Hence the use of the graphic-processing-unit (GPU) based parallel strategy appears to be a natural choice [23, 24]. In this study, we propose the utilization of FEM based quantitative PACT to derive the absolute optical absorption coefficient of the leaf in rice, which is positively relative to the concentration of chlorophyll. In addition, in order to improve the efficiency of the algorithm, a parallel computational strategy is implemented using a multicore graphics processing unit (GPU). Phantom experiments were carried out to
test the accuracy and efficiency of this method. The results show that our method is able to efficiently quantify the chlorophylls content accurately in plants and provide the distribution of the chlorophyll in leaves noninvasively.

2 Methods and materials

2.1 Experimental system

Fig. 1 shows the schematic of the PACT system. Briefly, an optical parametric oscillator (OPO) laser (Surelite OPO, Continuum, CA) pumped by a Q-switched Nd:YAG laser (Surelite I-20, Continuum, CA) emits laser pulses at a repetition rate of 20 Hz with a variable duration of 7–10 ns. The laser is re-directed by a reflection mirror (GCC-101102, Daheng Optics, Beijing), expanded using a combination of a concave lens (GCL-010911, Daheng Optics, Beijing) and a ground glass (OGW11-050, Zolix, Beijing), and delivered to the leaf fragment. Different from photosynthesis, the absorbed photons by the chlorophyll resulted in the temperature rise and further thermoelastic expansion which generated photoacoustic waves. The induced wideband photoacoustic signals are collected by a flat ultrasound transducer (V309-SU, Olympus) with a center frequency of 5 MHz and an aperture of 12 mm. The motorized rotator (RAP125, Zolix) scans the transducer along a circular trace with a diameter of 56 mm. The transducer collects a total number of 720 photoacoustic (PA) signals with an angular step of 0.5°. The PA signals are amplified at ∼39 dB using a low-noise amplifier (5073 PR, Olympus) and digitalized by a high-speed data acquisition card (PCI-5122, National Instruments). Before acquiring a PACT image, the laser energy was recorded for quantitative calculation [25].

![Figure 1: The schematic of PACT system; R: reflection mirror; C: concave lens; G: ground glass; T: transducer; Amp: amplifier.](image)
2.2 FEM based quantitative PAT reconstruction algorithm

There are three steps in the quantitative reconstruction method to determine the chlorophyll distribution in leaves. Fig. 2 shows the flow diagram of the method. The first two steps have been described in detail in our previous publications [26, 27]. We give a brief outline here. The first step is to obtain the map of absorbed optical energy density through a model-based finite element reconstruction algorithm. The algorithm is based on an iterative finite element solution to the photoacoustic equation starting from presumably uniform initial guess of optical and acoustic properties, while minimizing the weighted square errors between the measured and computed data using Newton-type method coupled with a hybrid scheme of Marquardt and Tikhonov regularizations. The core procedure can be described by the following two equations:

\[
\nabla^2 p(r,t) - \frac{1}{v_0^2} \frac{\partial^2 p(r,t)}{\partial t^2} = -\frac{\beta}{C_p} \Phi(r) \frac{\partial f(t)}{\partial t}, \tag{2.1}
\]

\[
(\mathcal{S}^T \mathcal{S} + \lambda I) \Delta \chi = \mathcal{S}^T (P_o - P^c), \tag{2.2}
\]

where \(p(r,t)\) is the photoacoustic pressure, \(v_0\) is the acoustic speed, \(\beta\) is the thermal expansion coefficient, \(C_p\) is the specific heat, \(\Phi(r)\) is the absorbed energy density that is the product of absorption coefficient \(\mu_a(r)\) and optical fluence \(\Psi(r)\) (i.e., \(\Phi = \mu_a \Psi\)), \(J(t) = \delta(t-t_0)\) is assumed in our study, \(P_o = (P_{o1}, P_{o2}, \cdots, P_{oM})^T\), \(P^c = (P_{c1}, P_{c2}, \cdots, P_{cM})^T\), and \(P_{o1}, P_{c1}\) are observed and computed acoustic field data for \(i = 1,2,\cdots,M\) boundary locations; \(\Delta \chi\) is the update vector for the absorbed optical energy density, \(\mathcal{S}\) is the Jacobian matrix formed by \(\partial p / \partial \Phi\) at the boundary measurement sites, \(\lambda\) is the regularization parameter determined by combined Marquardt and Tikhonov regularization schemes and \(I\) is the identity matrix. The second step is to recover the image of absorption coefficient from the absorbed energy density obtained in the first step based on the finite element solution to the photon diffusion equation:

\[
-\nabla \cdot D(r) \nabla \Psi(r) + \mu_a(r) \Psi(r) = q(r), \tag{2.3}
\]

where \(D = 1/ \left( \mu_a + \mu'_s \right)\) is diffusion coefficient, \(\mu'_s\) is the reduced scattering coefficient which is assumed as constant, \(q\) is the incident laser source. The distribution of the absorption coefficient \(\mu_a\) can be obtained by solving \(\mu_a = \Phi / \Psi\) iteratively, while a calibration with absorption-dominated acoustic phantom needs to be performed to determine the constant \(\xi\), which represents the relationship between the absolute pressure \(p_{real}\) and the measured temporal acoustic signals \(p_m\) [28]. \(p_{real}\) at the surface of a laser irradiated phantom can be approximately written as:

\[
p_{real} = \Gamma \mu_a \Psi_0 = \xi p_m, \tag{2.4}
\]

in which \(\Gamma\) is the Grueneisen coefficient (\(\Gamma = v_0 \beta / C_p\)), \(\Psi_0\) is the incident laser fluence at the surface of the phantom. Once \(\xi\) is determined, the reconstructed absorption coefficient in absolute units can be obtained. The last step is to quantify the distribution of the chlorophyll content from the absorption coefficient obtained in the second step. In most cases
for chlorophyll imaging, chlorophyll A and chlorophyll B are the two major absorbers. Using multispectral measurements, these two concentrations, $[\text{Chl.a}]$ and $[\text{Chl.b}]$ can be obtained using the following well-known relationship:

$$\mu_a(r, \lambda) = \varepsilon_a(\lambda)[\text{chl.a}] + \varepsilon_b(\lambda)[\text{chl.b}],$$

(2.5)

where $\varepsilon_a(\lambda)$ and $\varepsilon_b(\lambda)$ are the known molar extinction coefficient of chlorophyll A and chlorophyll B at wavelength $\lambda$. The total chlorophyll concentration can be calculated as $[\text{chl}] = [\text{chl.a}] + [\text{chl.b}]$. We also note that at the wavelength of 662 nm, the molar extinction of chlorophyll A is at least order higher than that of chlorophyll B. Therefore, in this case, we use the result at 662 nm to achieve an approximated concentration of chlorophyll A.

The parallel calculation in our study is based on a hardware and software architecture for general computing purpose on a GPU named the “compute unified device architecture” (CUDA), and this framework provides a low-cost, powerful tool for parallel calculation with a personal computer. In this work, we implemented the GPU-accelerated code using the CUDA C language based on the linear algebra library cuBLAS and cuSPARSE, which provide the linear algebra operations on matrix and vectors for dense and sparse linear systems. Single precision data type for all variables and parameters were applied in the code to reduce storage requirements and improve computational speed. A device interface was applied in order to manually transfer data and reduce unnecessary data communication between CPU and GPU. Fast shared memory was used to avoid accessing the global memory directly. Page-lock memory was used for achieving higher bandwidth between host and device. Based on the forward model discussed earlier and illuminated in Fig. 2, there are two main procedures that would be carried out for many
times: 1) assembling a new vector by the multiplication operation between a matrix and a vector; 2) solving the linear matrix equation. In this work, for the first procedure, we divided the matrix and vector into different kernels named as “blocks” and “threads” and applied the calculations simultaneously, which was a regular parallel strategy in GPU processing. When solving the PAE

\[ \mathbf{A}\mathbf{p}^{c,i} = B\Phi^i, \]  

we first calculated the inversion matrix of the global system matrix \( \mathbf{A} \) and then obtained the acoustic pressure \( \mathbf{p}^{c,i} \) by

\[ \mathbf{p}^{c,i} = \mathbf{A}^{-1}\mathbf{B}\Phi^i. \]  

Here we developed a new approach to achieve the inversion of the global system matrix \( \mathbf{A} \), which contains two steps: the Cholesky decomposition of the global system matrix

\[ \mathbf{A} = \mathbf{LL}^T, \]  

where \( \mathbf{L} \) is a low triangular matrix, and the solution to the matrix equation

\[ \mathbf{LL}^T \mathbf{A}^{-1} = \mathbf{I} \]  

using an iterative conjugate gradient solver with preconditioning. In the inverse model, the most time-consuming procedure in the GPU-accelerated code is the computation of the Jacobian matrix \( \mathbf{J} \) in Eq. (2.2). Instead of using several kernels to calculate each individual columns of the Jacobian matrix sequentially, we successfully assembled the whole Jacobian matrix \( \mathbf{J} \) in one time by making the use of the developed new approach to achieve the inversion of the global system matrix \( \mathbf{A} \). We furthermore improve the parallel degree of other parts in the inverse model using similar ways in the forward model and increase the computational efficiency dramatically.

### 2.3 Phantom and sample preparations

Phantom experiments were performed to validate and calibrate the algorithm. We mixed India ink and agarose with different ratio to simulate different optical absorption coefficients. The background has an optical absorption coefficient of 0.007 \( \text{mm}^{-1} \) and two round targets with a diameter of 4 mm have optical absorption coefficients of 0.028 \( \text{mm}^{-1} \), and 0.049 \( \text{mm}^{-1} \), which provide contrasts of 4 and 7 times stronger to the background. We carried out photoacoustic experiments for three independent groups of rice leaves. Each group has a total number of 20 samples resected from 20 plants. The rice leaves were cut into small squares and fixed on the surface of a cylindrical phantom using transparent agarose. The ultrasound transducer and the leaf were immersed in water for the coupling of PA signals. We extracted the concentrations of chlorophyll A in all rice leaves through a standard chemical extraction procedure as standard values for further quantitative comparison with reconstructed ones. The extraction solvent was mixed by analytical reagent acetone and anhydrous alcohol at a ratio of 2:1. Then the rice leaves were
cut into small strips with a maximum width of 1 mm. We immersed 0.2 g of each sample in 10 mL extraction solvent sealed in a test tube. All the test tubes were kept in a dark room under room temperature until the samples became white. Finally, we measure the concentrations of chlorophyll A using a spectrophotometer.

3 Results

As shown in Fig. 3, we first evaluated the reconstructed accuracy of the GPU-based code using phantom experiments. Figures 3a and 3e show the recovered geometry of the targets in different cases using the algorithm of delay and sum. Figs. 3b and 3f present the reconstructed results of the targets with given optical absorption coefficients of 0.028 mm$^{-1}$ and 0.049 mm$^{-1}$ using CPU-based code. Figs. 3c and 3g display the quantitatively reconstruction results using the proposed GPU-based code. We can see that the results from the CPU and GPU are almost the same. The error between these results are less than 0.1%. In addition, we quantitatively compared the reconstructed geometries and optical absorption coefficients to the given values for these two cases in Figs. 3d and 3h, indicating that the reconstructed parameters agree well with the exact values.

We further evaluated speed-up ratio of our GPU-accelerated code with these three sets of phantom data using different dual meshes and compared the reconstruction results with the existing CPU-based code. Table 1 lists the computational times using CPU and GPU codes with different meshes. All data was obtained after three iterations. The CPU used in this study is Intel i7-6700, while the GPU is Nvidia GeForce GTX Titan X. The

![Figure 3: Reconstructed optical absorption coefficient images for phantom experiments.](image-url)

(A, E) The results obtained by delay and sum algorithm. (B, F) The quantitative results obtained by FEM algorithm using CPU. (C, G) The quantitative results obtained by FEM algorithm using GPU. (D, H) Quantitative comparison between reconstructed values and exact values. Blue lines indicate the exact diameter and optical absorption coefficients, and red lines represent the reconstructed diameter and optical absorption coefficients.
Table 1: Performance comparison between GPU- and CPU-based reconstructions.

<table>
<thead>
<tr>
<th>Dual Mesh Pair</th>
<th>GPU (sec)</th>
<th>CPU (sec)</th>
<th>Speed-up Ratio</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>630-2457</td>
<td>12.2</td>
<td>515.5</td>
<td>42.2</td>
<td>&lt;0.1%</td>
</tr>
<tr>
<td>630-9705</td>
<td>71.2</td>
<td>6510.1</td>
<td>91.4</td>
<td>&lt;0.1%</td>
</tr>
<tr>
<td>1525-5977</td>
<td>89.0</td>
<td>10005.2</td>
<td>112.4</td>
<td>&lt;0.1%</td>
</tr>
<tr>
<td>3627-14325</td>
<td>496.6</td>
<td>71760.9</td>
<td>144.5</td>
<td>&lt;0.1%</td>
</tr>
</tbody>
</table>

Comparison in Table 1 shows that the GPU code significantly reduces the computational time compared to the CPU counterpart, especially for large mesh pairs. The speed-up ratio increased from 42.2-fold to 144.5-fold when the number of nodes in fine meshes increases from 2457 to 14325. In addition, the errors in all cases are less than 0.1%, which shows that the proposed single precision GPU-based code has the same accuracy with the conventional CPU-based code. Comparing with our previous work, the speed-up ratio is increased from 80 to 112.4 for the same case [23]. The first row of Figs. 4a, 4b, and 4c presents the photographs of typical rice leaves in three independent groups. We applied the GPU-based quantitative reconstruction code to derive the optical absorption maps of three independent rice groups A, B and C.
Figure 5: Relative quantitative comparison between reconstructed absorption coefficients and chemical extracted conventions of chlorophyll A in three independent groups of rice leaves.

chlorophyll A in the rice leaves. Before the quantitative reconstruction, we recovered the geometries of rice leaves using delay and sum algorithm as shown in the second row of Figs. 4a-4c. The last row represents the quantitative reconstructed maps of optical absorption coefficients. Both delay&sum and FEM-based algorithm are able to reconstruct the correct shape and size of rice leaves, which is consistent with the samples in photographs. In addition to geometries, our quantitative reconstruction method provides the distribution of chlorophyll A in rice leaves. Based on our quantitative reconstruction method, the distribution of optical absorption coefficients for chlorophyll A has been derived, which reflects the distribution of concentrations for chlorophyll A in leaves. The chemical extraction shows the total concentration of chlorophyll A in each sample, which is tightly associated with the sum of reconstructed optical absorption coefficients over the entire sample. Fig. 5 presents the relative quantitative comparison between the summed optical coefficients and chemical extracted concentrations for three independent groups. For both methods, we calculated the error bar for each group using Mean ± SEM, and normalized the values of three groups assuming that the values of the first group are 1. The reconstructed optical absorption coefficients in group 2 and 3 are consistent with the chemical extracted concentrations of chlorophyll A.

4 Discussion and conclusion

In summary, a GPU-accelerated FEM-based quantitative PACT reconstruction method for non-invasively mapping chlorophyll A in rice leaves is proposed in this paper. The efficiency and accuracy of this method are evaluated through a series of experiments from phantoms to rice leaves, and compared with traditional methods. The results in-
dicate that this method has similar accuracy to the traditional methods but overcomes many disadvantages such as time-consuming and background light susceptible. This method provides a promising tool for studying plant physiological state and process in the future. However, further improvements are needed to make it suitable for in vivo deriving concentrations of functional parameters in plant leaves with improved accuracy. First, in this study, we only used 662 nm, which is limited by the available tunable range of the laser in our lab. To derive more functional parameters such as chlorophyll A, chlorophyll B, carotenoids, and water with more accuracy, more wavelengths are required. In addition, a model, used to derive real concentrations of functional parameters based on maps of optical absorption coefficients, should be proposed [29]. Second, we need to scan the transducer in the current system setup since only one ultrasound transducer is employed. To achieve real-time imaging, a transducer array is preferred. Furthermore, a handheld configuration of the imaging interface will make it suitable for outdoor imaging of plant leaves in vivo. Finally, in the algorithm, the first step is to set an initial value. In our case, the initial value is arbitrary, thus more iterations are needed. If we can find a proper initial value, the calculation time will be significantly reduced with improvement in accuracy of reconstruction. One potential solution is to select a proper initial value based on we may the relative intensity distribution reconstructed by the delay and sum.

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